

Husimi Maps in Lattices

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We build upon previous work that used coherent states as a measurement of the local phase space and extended the flux operator by adapting the Husimi projection to produce a vector field called the Husimi map. In this article, we extend its definition from continuous systems to lattices. This requires making several adjustments to incorporate effects such as group velocity and multiple bands. Several phenomena which uniquely occur in lattice systems, like group-velocity warping and internal Bragg diffraction, are explained and demonstrated using Husimi maps. We also show that scattering points between bands and valleys can be identified in the divergence of the Husimi map.

I. INTRODUCTION

In Mason *et al.*[1], we introduced a new interpretation of the probability flux operator

$$\hat{\mathbf{j}}(\mathbf{r}) = \frac{1}{2m} (|\mathbf{r}\rangle \langle \mathbf{r}| \hat{p} + \hat{p} |\mathbf{r}\rangle \langle \mathbf{r}|) \quad (1)$$

by expressing its eigenstates as the limit of measurements by infinitesimally small coherent states. Our approach yields a new perspective on flux measurements and provides a novel tool for visualizing wavefunctions which parallel the probability flux map. Because they are based on the Husimi projection technique[2], these visualizations are called "Husimi maps". Husimi maps improve the understanding of the semiclassical paths underlying the quantum wavefunctions and can be of use even for systems where the traditional flux has little success (i.e., when it is either zero or strongly misleading). Later work[3] further developed the numerical framework of the Husimi map and applied it to a wider variety of systems by incorporating local potentials and examining flux through open systems.

This article expands the Husimi map technique from continuous, free-particle systems like the two-dimensional electron gas (2DEG) to crystalline systems like graphene. While the extended wavefunction of an electron in a crystal is continuous, the potential imposed by the nuclei can be modeled by replacing the continuum with localized wavefunctions centered at individual tight-binding lattice sites. These individual wavefunctions combine to form a model of the entire wavefunction, which now defines their envelope function. In this model, Eq. 1 describes not the probability flow at an infinitesimal point, but the flow of probability in and out of the localized wavefunction at a single site.

Lattice systems can behave very differently from continuous systems. For instance, the orientation of the group velocity vector, which dictates classical dynamics, can strongly diverge from the wavevector, which was the initial foundation of the Husimi projection. In fact, the group-velocity space can be so strongly restricted that classical trajectories are only permitted along certain directions, dramatically affecting the dynamics of states that inhabit lattice systems. When these trajectories hit

a boundary, internal Bragg diffraction can produce additional nonclassical ray reflections.

Here we explore two-dimensional square and honeycomb lattices; extension to three-dimensional systems is straightforward. Honeycombs induce an additional phenomenon: the presence of multiple bands and valleys, by which different quasiparticles can propagate and interfere. While the flux operator is unable to reflect any of these behaviors, in this article we show that with proper modifications, the Husimi projection can handle them with ease.

This paper is organized as follows: In Section II A we provide the definition of the Husimi projection for continuous system and then modify the Husimi projection in Section II C to represent the group velocity and multiple bands. In Section III A, we apply the Husimi projection to square lattices near the band center where group-velocity effects are strongest, and in Section III B, we examine the graphene honeycomb lattice. Finally, in Section III D, we provide an interpretation of unusual boundary reflections found in Sections III A and III B by demonstrating and measuring internal Bragg diffraction.

II. METHOD

A. Definition of the Husimi Projection

Building off work in Husimi[2] and Mason *et al.*[3], we define the Husimi function as a measurement between a wavefunction $\psi(\{\mathbf{r}_i\})$ and a coherent state $|\mathbf{r}_0, \mathbf{k}_0, \sigma\rangle$, which minimizes joint uncertainty in spatial and momentum coordinates. For lattice systems, the wavefunction represents the probability amplitude multiplier of localized wavefunctions indexed at discrete lattice sites, which are associated with discrete positions in the set $\{\mathbf{r}_i\}$. The coherent state is also an envelope function over localized wavefunctions, defined by the Gaussian function

$$e^{-(\mathbf{r}_i - \mathbf{r}_0)^2 / 4\sigma^2 + i\mathbf{k}_0 \cdot \mathbf{r}_i}$$

centered around \mathbf{r}_0 and \mathbf{k}_0 . The parameter σ defines the spatial spread of the coherent state and the uncertainties in space and momentum according to the well-known re-

lation

$$\Delta x \propto \frac{1}{\Delta k} \propto \sigma. \quad (2)$$

As a result, there is a trade-off for any value of σ selected: for small σ , spatial resolution is improved at the expense of resolution in momentum space, and vice versa for large σ .

We can explicitly write out the projection of the wavefunction onto the coherent state as

$$\begin{aligned} \langle \psi | \mathbf{r}_0, \mathbf{k}_0, \sigma \rangle &= \left(\frac{1}{\sigma \sqrt{\pi/2}} \right)^{d/2} \\ &\times \sum_i \psi(\mathbf{r}_i) e^{-(\mathbf{r}_i - \mathbf{r}_0)^2 / 4\sigma^2 + i\mathbf{k}_0 \cdot \mathbf{r}_i}, \end{aligned} \quad (3)$$

where d is the number of dimensions in the system. The Husimi function is then defined as

$$\text{Hu}(\mathbf{r}_0, \mathbf{k}_0, \sigma; \psi(\{\mathbf{r}_i\})) = |\langle \psi | \mathbf{r}_0, \mathbf{k}_0, \sigma \rangle|^2. \quad (4)$$

If we weight the Husimi function by the central wavevector \mathbf{k}_0 , we obtain the Husimi vector. When momentum space is explored at a point by many Husimi vectors, the result is the full Husimi projection.

If all the Husimi vectors at a point are summed, the Husimi function can be used to construct and generalize the flux operator, resulting in the vector-valued function $\mathbf{Hu}(\mathbf{r}_0, \sigma; \psi(\{\mathbf{r}_i\}))$ equal to

$$\mathbf{Hu}(\mathbf{r}_0, \sigma; \psi(\{\mathbf{r}_i\})) = \int |\langle \psi | \mathbf{r}_0, \mathbf{k}_0, \sigma \rangle|^2 \mathbf{k}_0 d\mathbf{k}_0. \quad (5)$$

Earlier work has shown that for $\sigma k \ll 1$, Eq. 5 is proportional to the traditional flux vector expectation value [3]. For lattice systems, the traditional flux becomes a finite-difference approximation defined by the lattice.

B. The Hamiltonian

This paper examines Hamiltonians using the nearest-neighbor tight-binding approximation

$$H = \sum_i \epsilon_i \mathbf{a}_i^\dagger \mathbf{a}_i - t \sum_{\langle ij \rangle} \mathbf{a}_i^\dagger \mathbf{a}_j \quad (6)$$

where \mathbf{a}_i^\dagger is the creation operator at orbital site i and we sum over the set $\langle ij \rangle$ of nearest neighbors. The quantity ϵ_i is the on-site energy and t is the hopping energy scale. For the square lattices, we set $\epsilon = -4t$. For systems at energies $E < 0.5t$, the tight-binding Hamiltonian is a close approximation to the effective mass envelope function Hamiltonian $H = -\frac{p^2}{2m} + U(\mathbf{r})$ where $t = \hbar^2/(2m^*a^2)$ and a is the mesh lattice spacing. For the honeycomb lattice, parameters are set to the common values in the literature for graphene: $\epsilon = 0$ and $t = 2.7\text{eV}$ [4, 5]. Eigenstates of closed stadium billiard systems are computed using the standard sparse matrix eigensolvers.

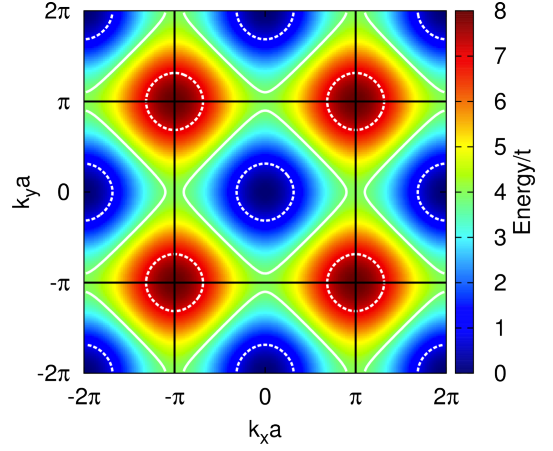


Figure 1: The two-dimensional dispersion relation for the square lattice demonstrates strong group-velocity warping at the band center ($E = 4t$). The dispersion relations for $E = 0.9t$, and $7.1t$ (dashed white lines) are nearly circular, while the relation near the band edge at $E = 3.9t$ (solid white lines) shows strong warping.

C. Group Velocity

In the original introduction of the Husimi map[3], each Husimi function is weighted by the wavevector of the coherent state to produce a visual guide to the classical dynamics of the system. Summing all the vectors equates to the flux operator (Eq. 5) when the coherent states are sufficiently small. This equivalence holds in lattices, however, the direction and magnitude of the group velocity $\nabla_{\mathbf{k}} E(\mathbf{k})$ can strongly diverge from the wavevector. Since a coherent state, which is now defined as an envelope function over localized wavefunctions, follows the group-velocity vector instead of its wavevector, it is necessary to weight the Husimi function by group-velocity vectors to indicate the classical dynamics. As a result, the Husimi projection indicates the classical flow of quasiparticles, in contrast to the flux operator (Eq. ??), which instead indicates the flow of probability.

At low energies, the square lattice closely approximates a free-particle continuous system so that this modification is minimal. At higher energies, however, the mapping from the wavevector to group velocity can be strongly constricted. For example, at energies near the band center of $E = 4t$, there are only four directions available to the group velocity in the square lattice, as shown in the solid white contour in Fig. 1 at $E = 3.9t$.

To visualize this effect, we show group-velocity Husimi projections at three representative energies in Fig. 2 for the square lattice. Thirty-two equally-spaced angles along a circle are chosen to represent the local momentum space. Wavevectors are chosen with these angles to satisfy the dispersion relation for a given energy.

At energies away from the band center for the square lattice, semi-classical trajectories can assume any direction, but near the band center they must follow pre-

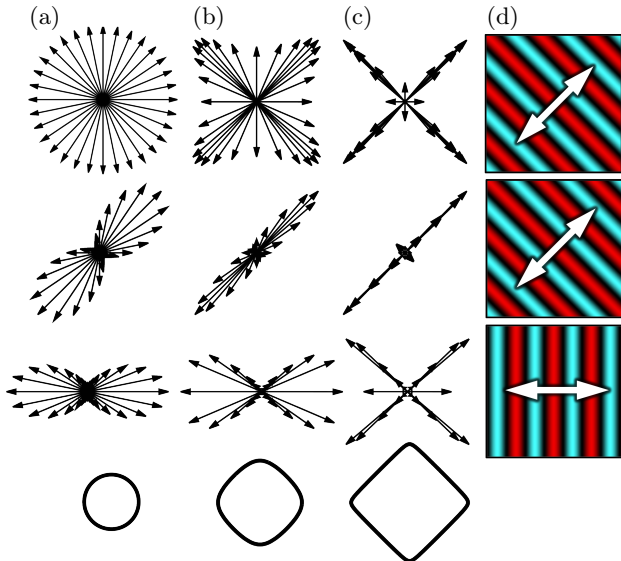


Figure 2: The group-velocity Husimi projection for the square lattice is strongly affected by warping at energies near the band center (Fig. 1). Husimi projections are shown for the square lattice for the group-velocity representation at $E = 0.9t$ (a), $3.0t$ (b), and $3.9t$ (c) with relative uncertainties of $\Delta k/k = 2$ (top) and 50% (middle and bottom). A schematic of the dispersion relation contour at each energy is shown at the far bottom. The generating wavefunction ψ for each row is shown in (d). In the top and middle row the test wavefunction is a cosine wave pointing along the 45° diagonal, and in the bottom along the 0° horizontal.

ferred directions determined by the group-velocity warping. However, the manner in which they do so may differ. This can be seen in Fig. 2 which examines two cosine-wave states with different wavevectors. As the energy of the system increases from left-to-right, group-velocity warping draws Husimi vectors, and the classical paths, towards four preferred directions. When the generating wavevector points along one of these directions, group-velocity warping merely sharpens the profile. When the generating wavevector points *in between* the preferred directions, as in the bottom row of Fig. 2, the classical trajectories are more strongly dependent upon the system energy.

Any expectation value over a wavefunction must be evaluated, usually by an integral, over a complete basis. As a result, any expectation value derived from the Husimi projection must be first computed from the wavevector basis; modifications to account for group velocity are determined afterwards. For instance, in the Multi-Modal Algorithm, which approximates the full Husimi projection by a subset of local plane waves (see Mason *et al.*[3] for more details), each approximation is achieved by computing the dot product between the Husimi projection and template projections in k -space. Because of group-velocity warping, the resulting wavevectors no longer indicate classical flow. To address this problem, the resulting dominant wavevectors

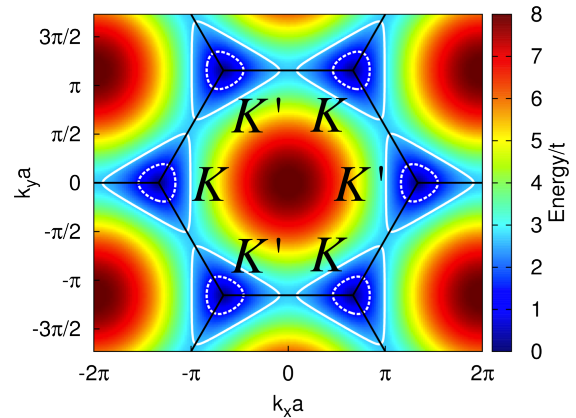


Figure 3: Like the square lattice in Fig. 1, the two-dimensional dispersion relation for the honeycomb lattice demonstrates strong group-velocity warping at energies away from the Dirac point. The dispersion relation for $E = 0.5t$ (dashed white lines) is nearly circular, while the relation at $E = 0.98t$ (solid white lines) shows strong warping. The K and K' valleys are indicated.

are then mapped onto group velocity by taking the local derivative of the dispersion relation.

D. Band Structure

The number of bands for a lattice system is equal to the number of tight-binding orbitals in the unit cell[6]. The square lattice has only one unique tight-binding orbital and only one band, but due to the warping in the band structure, distinct behaviors result at energies above $E = 4t$, corresponding to the hole pocket (see the contour lines in Fig. 1 near the corners of the Brillouin zone). However, because the quadratic dispersion relations at $E = 0$ and $E = 8t$ are separated by energy, a semi-classical interpretation of a wavefunction is always constrained to one relation or the other.

In the honeycomb lattice, however, there are *two* unique orbitals in the lattice structure, yielding two bands that touch at the Dirac point at $E = 0t$. But more interestingly, the band structure warps each band to produce the inequivalent K and K' valleys at the Dirac point, which are indicated in Fig. 3. Unlike the square lattice, these two valleys co-exist in the energy range $-t < E < t$.

These valleys exhibit a linear dispersion relation near the Dirac point[4]. At energies away from the Dirac point, the two valleys undergo group-velocity warping that emphasizes three directions, which is referred to as “trigonal warping”[5]. The effects of trigonal warping can be significant even at energies as low as $0.2t$.

The Husimi map can assist visualizations of intervalley scattering, the scattering of quasiparticles between the two valleys which are part of the same band. To resolve the two valleys, it is simply necessary that the uncer-

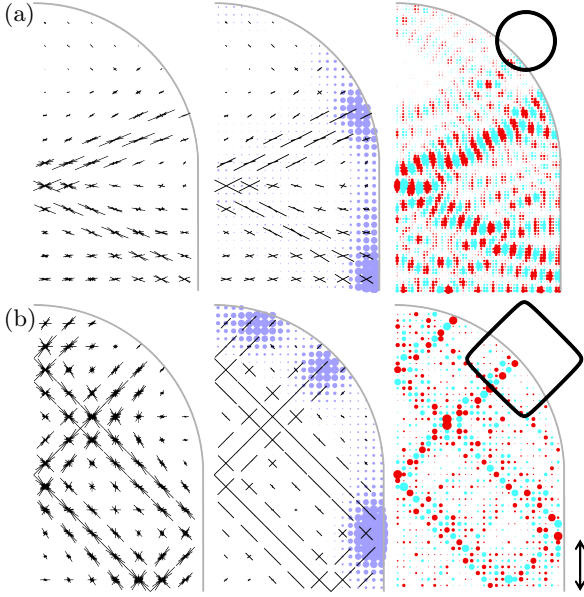


Figure 4: The full wavevector Husimi map (left), multi-modal analysis (middle) and wavefunction (right) for two stadium eigenstates at energies $E_1 = 1.496t$ (a) and $E_2 = 3.982t$ (b) (a schematic of the dispersion relation contour at each energy is shown in the insets). The uncertainty for each projection is set to $\Delta k/k = 10\%$, and the spread of the coherent state is indicated by double arrows on the right. Angular deflection (Eq. 8) is indicated in blue. Each eigenstate has similar characteristic wavelengths, but the lower eigenstate is sampled with half the linear resolution, causing its energy to go up and the group velocity to become more restrictive.

tainty of the coherent state is small enough in k -space to unambiguously resolve the wavevectors of each valley. Because the two valleys of graphene are well-separated and only come close at the corners of each triangle in Fig. 3, the Husimi projection can clearly resolve the two valleys at most energies. More complicated lattices can have additional bands, and any automated method for calculating Husimi maps for these systems have to take their mutual distance in k -space into account.

III. RESULTS

A. Stadium Billiard Eigenstates of the Square Lattice

In Fig. 4, we examine two closed stadium billiard systems with identical geometric parameters. Both systems are created using the square-lattice tight-binding model, but the lattice constant in Fig. 4b is twice as large, so the system possesses far fewer sampling points and experiences stronger effects from group-velocity warping. These systems connect to the lattice-sampled Schrodinger equation for a continuous system, which can avoid the effects of group-velocity warping by increasing

the number of sample points in the system (See Fig. 4). However, lattice spacing is not an adjustable parameter in atomic systems, and group velocity must be given careful attention.

Keeping the characteristic wavelength constant raises the energy in any system with a longer lattice constant. In Fig. 4b, an eigenstate of the system is shown with energy $E_2 = 3.982t$, near the band center. The energy for the system in Fig. 4a is chosen to reflect the same characteristic wavelength, which depends upon which direction in k -space is considered. Along the k_x -axis, the energy is bounded below by $\frac{E_2}{t_2} = -2 \left(\cos \left(\frac{a_2}{a_1} \cos^{-1} \left[1 - \frac{E_1}{2t_1} \right] \right) - 1 \right)$, and at 45-degrees from the k_x -axis, it is bounded from above by $\frac{E_2}{t_2} = -4 \left(\cos \left(\frac{a_2}{a_1} \cos^{-1} \left[1 - \frac{E_1}{4t_1} \right] \right) - 1 \right)$. By setting $\frac{a_2}{a_1} = \frac{1}{2}$ and $t_1 = t_2 = t$ an eigenstate is chosen with an energy near the average of the bounds at $E_1 = 1.496t$.

The classical trajectories indicated by the Husimi map in the low-energy state in Fig. 4a point along directions oblique to the 45° diagonals and intermingle among other paths at other angles. The Husimi map for the higher energy eigenstate in Fig. 4b instead *only* indicates classical trajectories along the 45° diagonals. Moreover, the trajectories in the higher-energy system are much clearer since they are reinforced by a restricted group-velocity space.

The Husimi map makes it possible to measure “angular deflection”, which reflects how classical trajectories deviate from the straight line in response to the system. Angular deflection thus provides a map of where the boundaries or external potentials most strongly effect these dynamics, and can be interpreted as a force on the particle represented by the wavefunction.

For lattice systems, the original definition of angular deflection provided in Mason *et al.*[3] must be modified to account for group velocity. It can thus be defined

$$Q_{\text{ang.}}(\mathbf{r}; \Psi) = \int D_{\text{abs.}}(\mathbf{r}, \mathbf{k}; \Psi) |\nabla_{\mathbf{k}} E(\mathbf{k})| d^d k, \quad (7)$$

where the quantity $\nabla_{\mathbf{k}} E(\mathbf{k})$ represents the group-velocity vector corresponding to the wavevector \mathbf{k}' , and the integral covers all wavevectors satisfying the dispersion relation. The quantity $D_{\text{abs.}}(\mathbf{r}, \mathbf{k}; \Psi)$ is defined as the Gaussian-weighted absolute divergence of the Husimi function for one particular trajectory angle

$$D_{\text{abs.}}(\mathbf{r}, \mathbf{k}; \Psi) = \int \sum_{i=1}^d \left| \frac{\text{Hu}(\mathbf{k}, \mathbf{r}'; \Psi) - \text{Hu}(\mathbf{k}, \mathbf{r}; \Psi)}{(\mathbf{r}' - \mathbf{r}) \cdot \mathbf{e}_i} \right| \times \exp \left[-\frac{(\mathbf{r}' - \mathbf{r})^2}{2\sigma^2} \right] d^d r', \quad (8)$$

where we sum over the d orthogonal directions each associated with unit vector \mathbf{e}_i .

Fig. 4 shows angular deflection in blue, concentrated on the boundary as expected. Because the resolution of

angular deflection is limited by the spread of the coherent state used for Husimi sampling, its spread into the bulk from the boundary exhibits the same Gaussian distribution that is used for the test wavepacket. It is worth noting that without the proper modifications, angular deflection based on the wavevector shows non-trivial results in the bulk of the system even when there are no external fields.

This also suggests that modifications may be in order for other metrics for lattice systems. For instance, by coordinating the boundary divergence with each wavevector, one can compute the quantum analog of a state's Poincare map[7]. In Birkhoff coordinates[8, 9], the angle of impact is mapped against a coordinate along the boundary, and both fully quantum[10, 11] and classical[12] variations have become valuable tools in quantum chaos. By incorporating group-velocity considerations, these metrics may be extended to lattice systems.

B. Stadium Billiard Eigenstates of the Honeycomb Lattice

For the square lattice, time-reversal symmetry is expressed in the Husimi projection by the fact that each Husimi vector is accompanied by another of equal magnitude but opposite direction. This causes the flux operator and Eq. 5 to return null results. The same is true for the honeycomb lattice, except that the range of wavevectors available at low energies point towards the K and K' valleys.

But when the Husimi vectors are weighted by the group-velocity and not the wavevector, a different behavior emerges. In the honeycomb lattice, group-velocity doesn't correlate at low energies with \mathbf{k} but $\mathbf{k} - \mathbf{K}^{(\prime)}$. If one examines the Husimi projection for each valley individually, it is no longer true that each Husimi vector is accompanied by its opposite. Rather, each valley is the time-reversal symmetric version of the other, allowing Husimi vectors in each valley to sum to non-trivial results.

Fig. 5a shows the Husimi map of the K' valley for a high-energy eigenstate in part (b) where the strong pull towards the three preferred group-velocities is evident. In parts (c) and (d), the multi-modal analysis for the K' and K valleys are shown. According to the time-reversal symmetric relation, the Husimi map for the K valley is the precise inverse of the K' valley. While the classical trajectories are evident in the wavefunction (Fig. 5b), the Husimi map identifies their orientation for each valley.

Because Husimi vectors for each valley no longer sum to zero, it is possible to produce divergence in the Husimi map for each wavevector. This is identical to angular deflection in Eq. 8 except that the absolute value is not taken in the integrand. And like angular deflection, the integrand must be weighted by the group-velocity vector, or non-trivial results emerge in the bulk of the system.

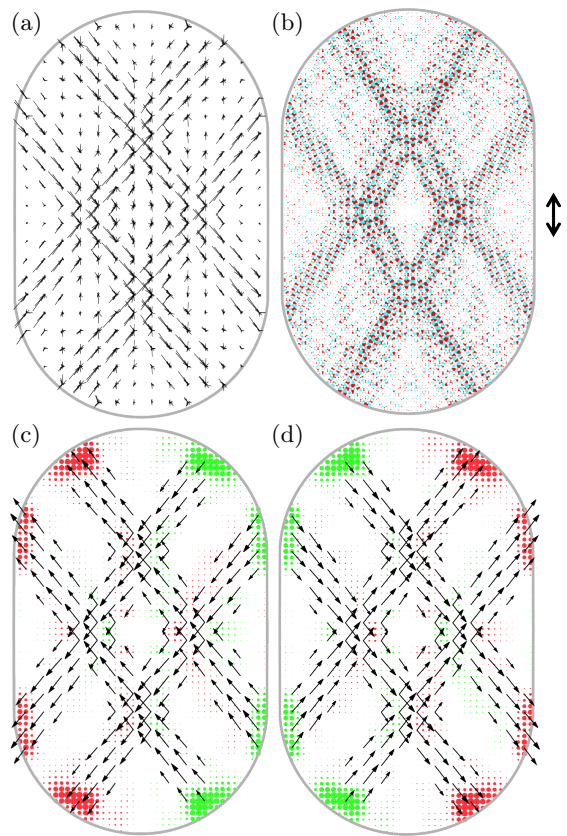


Figure 5: The full Husimi map around the K' valley(a), the wavefunction(b), the multi-modal analysis for the K' valley(c) and for the K valley(d) for a high-energy eigenstate of the honeycomb lattice at $E = 0.786t$. This system is a closed stadium billiard system with 20270 lattice points. The relative uncertainty in all calculations is $\Delta k/k = 20\%$ with the coherent state spread indicated by the double-arrows. Because of time-reversal symmetry, the Husimi maps in (c) and (d) are exact inverses of each other. Unlike the square lattice, the summing the Husimi vectors for each valley in a honeycomb lattice gives non-zero results for a closed system, giving rise to non-trivial divergences along the boundary where one valley scatters into the other (indicated in green for positive and red for negative).

Summing the divergence for all wavevectors produces the total divergence, which appears in green and red in Figs. 5c and 5d to indicate positive and negative values. These points are, in fact, sources and drains for each valley, and represent the inter-valley scattering points along the boundary, whose scattering properties depend on the angle of the cut[13]. The results in Fig. 5 suggest that each classical trajectory in this wavefunction shares half of its existence in one valley, and half in the other.

C. Group Velocity Warping

This section expands upon our findings in Figs. 4 and 5 by examining Husimi projections in detail. In Fig. 6, we

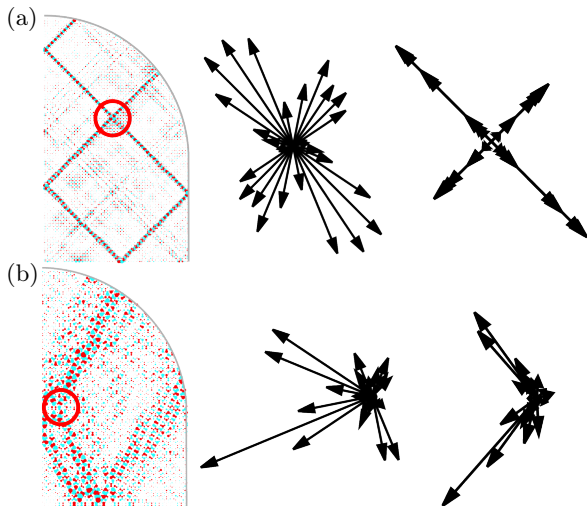


Figure 6: Two stadium eigenstates for the square lattice (a) and the honeycomb lattice (b). The wavefunctions (left), wavevector Husimi (middle) and group-velocity Husimi (right) projections are shown for the points circled in red. Uncertainties for both projections are $\Delta k/k = 20\%$. Not only is there more spread to the wavevector projections, these projections also indicate markedly different trajectory paths than the group-velocity equivalents. Moreover, the group-velocity projections are more consistent with the paths indicated by the wavefunctions.

show Husimi projections for the square (a) and honeycomb (b) lattices in both wavevector and group-velocity representations. As expected, the spread of each Husimi projection is dramatically reduced in the group-velocity representation, a consequence of group-velocity warping and consistent with Fig. 2. Moreover, a close examination reveals that Husimi wavevectors can point along surprisingly divergent angles from their trajectories, emphasizing the extent to which group-velocity warping establishes such states.

If it is possible to produce similar classical trajectories using a wider variety of wavevectors for lattices, then how are wavevectors distributed in this wider range? We can provide an answer by summing the Husimi projections over a range of eigenstates. We find that with a sufficient range of eigenstates, neither wavevector nor group-velocity distributions vary across the bulk of the system, except along the boundaries. For the square-lattice billiards, directions parallel to boundaries are emphasized, which is consistent with Dirichlet boundary conditions. This occurs even for jagged edges that do not fall along a symmetry axis of the underlying lattice.

Boundaries on the honeycomb lattice emphasize either parallel trajectories for intra-valley scatterers (zig-zag) or perpendicular trajectories for *inter*-valley scatters (arm-chair). We find that honeycomb lattice systems are more sensitive than the square lattice to the set of states we sum over, requiring a larger sum to provide uniform results. The distance from the edge where the emphasis occurs is a function of the characteristic wavelength; for

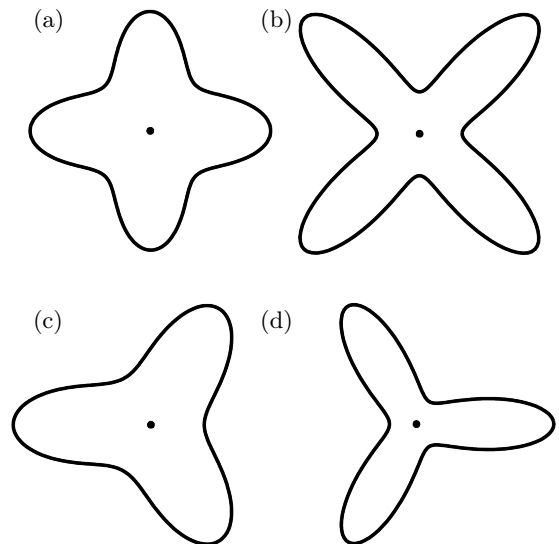


Figure 7: The distribution of Husimi vectors from the red circles in Fig. 6, summed over hundreds of eigenstates near $E = 3.5t$ for the square lattice and $E = 0.8t$ for the honeycomb lattice, with a coherent wavepacket spread of $\Delta k/k = 10\%$. Above, the wavevectors in the square lattice (a), group-velocities in the square lattice (b), wavevectors for the K' valley in the honeycomb lattice (c), and group-velocities for the K' valley in the honeycomb lattice (d). Husimi projections tend to emphasize wavevectors away from the preferred group-velocity directions (a,c), but not enough to overcome that preference in the group-velocity distribution.

the square lattice, this is k and in the honeycomb lattice $q = |\mathbf{k} - \mathbf{K}'|$. As a result, for small enough honeycomb systems, the emphasis of directions along the boundary can persist into the bulk.

In Fig. 7, we show a representative distribution of the wavevectors and group-velocities at the points circled in red in the stadium systems presented in Fig. 6, using Husimi projections with a coherent spread of $\Delta k/k = 10\%$. The states used for the square-lattice system are near energies of $E = 3.5t$, and at $E = 0.8t$ for the honeycomb lattice. More details can be found in Appendix A. Fig. 7 shows that the distribution among wavevectors emphasizes directions *away* from the preferred directions in group velocity. For certain energy regimes, *neither* wavevectors *nor* group velocities are evenly distributed across all eigenstates of a lattice system.

D. Internal Bragg Diffraction

The high-energy eigenstates from Fig. 6 exhibit an unusual behavior: the self-looping classical trajectories that are strongly emphasized in the wavefunctions do not exhibit specular reflection at the boundary. We clarify these reflections in the schematics in Fig. 8. Even though the absolute angles at each reflection point fall along the

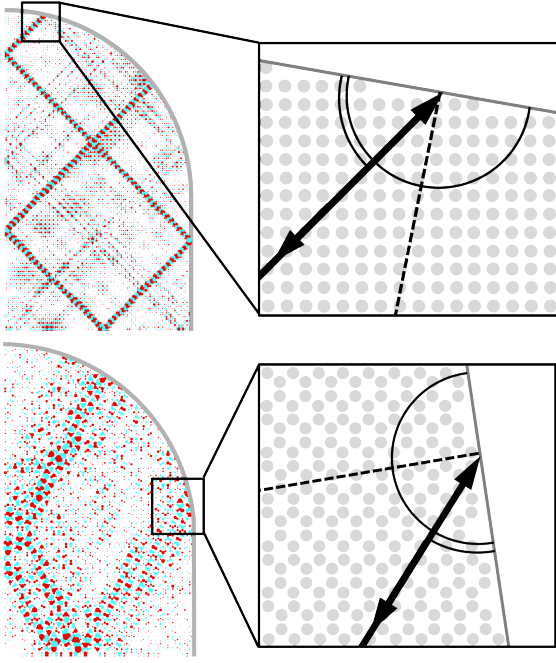


Figure 8: High-energy states in the square (a) and honeycomb (b) lattices can exhibit unusual behaviors, such as group-velocity warping and non-specular boundary reflections. The former can be seen in the wavefunction (left) by the restriction of trajectories to 45° diagonals for the square lattice (a) and the 60° diagonals for the honeycomb lattice (b). Non-specular reflections are magnified in the schematic (right). Even though the absolute incoming and outgoing angles for each point are the same angle, their angles of incidence (single and double arcs) are strongly divergent.

same diagonal, the *angles of incidence* vary substantially between the incoming and outgoing rays. In the honeycomb eigenstate (Fig. 8b), the reflection consists of scattering into the other valley and propagating in the exact opposite direction.

While the reflections of many trajectories in high-energy states violate specularity as a result of group-velocity warping, we have chosen the states in Figs. 6 and 8 specifically because these reflections behave in unexpected ways. Moreover, these surprising reflections occur only at certain points along the boundary where the lattice cut deviates from an axis of symmetry; specifically, they occur slightly off of clean cuts where jaggedness is most prominent.

To understand these unusual reflections, we use a technique called the Gaussian beam[14], which shows the entire set of wavefunctions available to the system which intersect at a particular point in both spatial and momentum coordinates. This is accomplished by weighting the eigenstates $\{\psi_E\}$ for a closed system by a coherent state $|\mathbf{r}_0, \mathbf{k}_0, \sigma\rangle$ which satisfies the dispersion relation at energy E_0 . To examine reflections at jagged boundaries, we place \mathbf{r}_0 along one of these boundaries and \mathbf{k}_0 point-

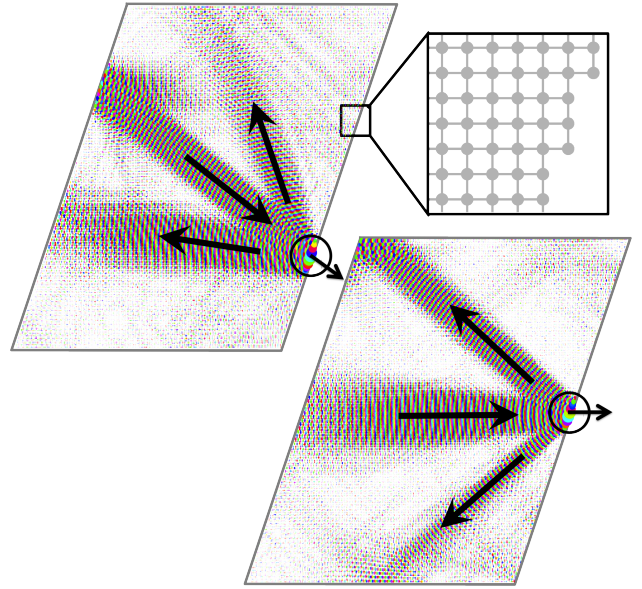


Figure 9: Two Gaussian Beams, constructed by summing the set of closed-system eigenstates in the energy range $2.48 < E < 2.52$ weighted by Eq. 9, using a coherent state with momentum uncertainty $\Delta k/k = 5\%$ that sits on the right-hand boundary (black circles) with specified momentum (small black arrows). The system is a square lattice cut at an 18° angle (inset). The incoming group-velocity angle is set to 0° at top and -40° at bottom.

ing away from the bulk. Each eigenstate is associated with an eigenenergy E so that the Gaussian beam Ψ is defined as

$$\Psi = \sum_E \langle \psi_E | \mathbf{r}_0, \mathbf{k}_0, \sigma \rangle \psi_E. \quad (9)$$

Because of the finite uncertainty of the coherent state, only wavefunctions at energies close to E_0 contribute to the final result. Thus, only a finite range centered around E_0 must be considered.

It is important to choose the spread of the coherent state wisely. Too large a coherent state restricts the set of eigenstates that contribute to the sum, giving unclear results. Too small a coherent state does not provide enough information to resolve features of the beam. In Fig. 9 a compromise is chosen at $\Delta k/k = 5\%$, which provides a sufficient range of eigenstates to construct a clear beam.

The classical paths suggested by the Gaussian beams in Fig. 9 must all travel through the position \mathbf{r}_0 with momentum $\hbar \mathbf{k}_0$ (Eq. 9) defined by the coherent state for each beam. In both top and bottom figures, the coherent state lies along the right-hand boundary, although the wavevectors for each coherent state differs. Because the breadth of a coherent state grows in time when it propagates, each beam focuses at the coherent state, and spread from its center. In both Figs. 9a and 9b, a specular reflected beam is present, but an additional reflected beam emerges as a result internal Bragg diffraction[15]. These additional reflections also appear

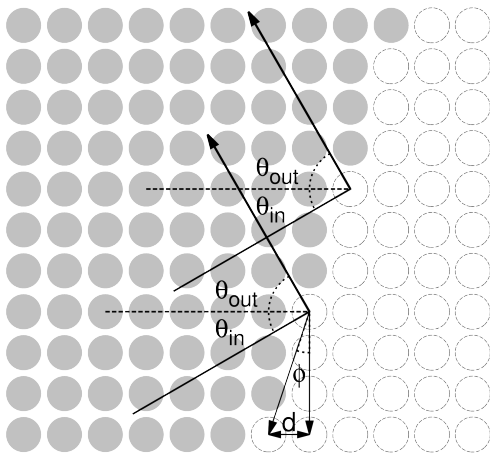


Figure 10: Schematic of internal Bragg diffraction. In light gray are the lattice sites for the system, and in dashed outlines are shown phantom lattice points outside the system where the wavefunction must go to zero. A ray coming in at an angle θ_{in} and reflects at θ_{out} interferes with rays from adjacent equivalent points on the boundary unit cell. The angle ϕ and horizontal distance between adjacent unit cells d are identical to the boundary in 9.

at scattering points for the square lattice in Fig. 8a.

It is possible to quantify internal Bragg diffraction by considering an edge identical to the system in Fig. 9 and depicted schematically in Fig. 10. Here the boundary is cut at an angle $\phi \approx 18^\circ$, where $\phi = 0$ is a vertical edge, and an incoming plane wave strikes the surface at angle θ_{in} , where $\theta_{in} = 0$ points to the right, and positive angles point upward. This plane wave reflects to an outgoing angle θ_{out} where $\theta_{out} = 0$ points to the left and positive angles point upward.

If there is a repeating unit cell in the edge, two rays which hit equivalent points of adjacent boundary unit cells gain or lose relative phase based on their wavevectors and the different distances they travel. For instance, a ray incurs an additional phase of $\delta = kd \frac{\sin(\theta - \phi)}{\sin \phi}$ when $\theta_{in} > -\phi$ and $\delta = kd \frac{\sin(\theta + \phi)}{\sin \phi}$ when $\theta_{in} \geq \phi$. Here d is the horizontal distance between identical points in adjacent unit cells and k is the wavevector magnitude of the incoming wave. When the plane wave is reflected, its neighbor gains phase according to the above formulas, but with k indicating the outgoing wavevector magnitude. When these two phases cancel or add to a multiple of 2π , the two rays constructively interfere. Since this is repeated over many unit cells, the interference can be quite strong.

Because the wavelength shrinks with increasing energy, more Bragg branches appear as energy goes up. And because the distance between adjacent unit cells increases for slighter angles against an axis of symmetry, more Bragg branches appear for shallower cuts. We find that both of these criteria are satisfied for the reflection points in Figs. 8 and 5.

Using the above formulas, we can predict internal

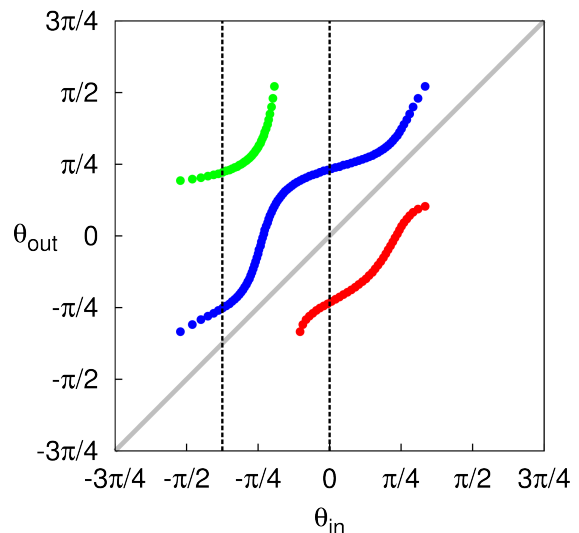


Figure 11: The internal Bragg relationship for a square lattice with an 18° cut as depicted in Figs. 9 and 10, computed using a scattering matrix on a square-lattice with 50 vertical unit cells at energy $E = 2.5t$. The identity line is shown in grey. The two incoming group-velocity angles from Fig. 9 of 0° and -40° are shown in vertical black dashed lines. The specular line is shown in blue, and the upper and lower branches are shown in green and red respectively.

Bragg diffraction for arbitrary cuts and energies. In Fig. 11, we present these results for the system in Fig. 9. The boundary unit cell consists of three vertical units and one horizontal unit, so that $\phi \approx 18^\circ$. The two incoming beams from Fig. 9 are represented by vertical dashed lines in Fig. 11. Each intersects the graph at the three locations: along the identity line for the incoming beam, along the blue specular line for an outgoing beam, and along one of the Bragg branches for the other outgoing beam. Our predictions are strongly validated by Fig. 9.

The σ spread of the test wavepacket used to create the Gaussian beam only covers 4 steps along the cut, meaning that only a few surface defects can produce substantial Bragg scattering. The ubiquity of this effect has implications for ray-tracing methods, which bridge classical and quantum explanations for phenomena such as fractal conductance fluctuations[16, 17] and caustics[18, 19] and encourages a re-examination ray-splitting[20] and other hypothetical edge effects[21, 22].

Combining group-velocity restriction and internal Bragg diffraction, we argue that the dense linear paths in the wavefunctions in Figs. 6 and 8 are indeed linked to classical rays which bounce back and forth approximately linearly; at one boundary the bounce is non-specular due to the cut of the edge and internal Bragg diffraction. For the honeycomb lattice, each bounce can be additionally associated with scattering into another valley. For both systems, these wavefunction enhancements are not strictly scars[23], which are generated by unstable classical periodic orbits in the analogous classical limit (group

velocity) system. Instead, the wavefunction structures are likely normal quantum confinement to stable zones in classical phase space.

IV. CONCLUSIONS

We have expanded the vector Husimi projection technique, introduced in Mason *et al.*[3], from the continuous system to lattices. We have demonstrated and explained two unusual properties of lattice systems using the Husimi projection: group-velocity warping and internal Bragg diffraction, both of which can strongly affect the properties of classical dynamics of these systems, in particular producing unexpected self-looping trajectories most visible in extreme-energy states. We have also shown that Husimi projections can isolate multiple bands which are simultaneously represented in the wavefunction, using the two valleys of the honeycomb as an example. For the honeycomb lattice, we have shown that one can identify locations of scattering between valleys by measuring the divergence of the Husimi map for each valley separately.

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Appendix A: Wavevector and Group Velocity Distributions

The plots in Fig. 7 are produced by summing the Husimi vectors over many eigenstates of each system in Fig. 6: For the square lattice, 600 states with energies $3.46t < E < 3.54t$ and for the honeycomb lattice, 300 states with energies $0.76t < E < 0.84t$. This is done for 256 wavevectors equally separated by angle, and then a small Gaussian kernel is applied with angle width $\pi/32$. Each Husimi vector is multiplied by the infinitesimal dk determined by the average distance to neighboring vectors in the sample, and each calculation takes place at the points circled in red in Fig. 6 with coherent spread of $\Delta k/k = 10\%$. The contour line in the dispersion relation is re-computed for each eigenstate to generate the coherent states for the Husimi projection. This is done to ensure that the steeper gradient of the dispersion relation near the preferred group velocities does not affect our results.

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